

Formation and dynamics of many-boson fragmented states in attractive one-dimensional ultra-cold gases

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Abstract

Dynamics of attractive ultra-cold bosonic clouds in one dimension are studied by solving the many-particle time-dependent Schrödinger equation. The initially coherent wave-packet can dynamically dissociate into two parts when its energy exceeds a threshold value. Noticeably, the time-dependent Gross-Pitaevskii theory applied to the same initial state does not show up the splitting. We call the split object *fragmenton*. It possesses remarkable properties: (1) it is two-fold fragmented, i.e., not coherent; (2) it is dynamically stable, i.e., it propagates almost without dispersion; (3) it is delocalized, i.e., the two dissociated parts still communicate with one another. A simple static model predicts the existence of fragmented states which are responsible for formation and dynamics of fragmentons.

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Dynamics of attractive low-dimensional dilute Bose gases have attracted much attention [1, 2, 3, 4, 5, 6, 7]. The formal equivalence of the Gross-Pitaevskii (GP) equation used to describe these quantum gases and the non-linear Schrödinger equation used in non-linear optics has led to transfer of knowhow and, most importantly, to the prediction of bright solitons in attractive Bose gases [1, 2]. More recently, fascinating and challenging experiments on bright matter-wave solitons have been reported [3, 4] and explained using GP theory, making attractive Bose gases a cornerstone of GP theory. Nowadays, the GP theory is widely utilized to study attractive dilute Bose gases.

GP theory is a mean-field approximation to the quantum *many-boson* problem, in which the Bose system is assumed to remain *condensed* during its evolution in time. Recently, the general validity of this assumption has been questioned in the theoretical study on dynamical depletion of attractive one-dimensional (1D) Bose systems at non-zero temperatures [8]. In the present Letter we consider the dynamics of attractive 1D Bose systems from the full many-body point of view and relate the many-body and GP results. We shall see that the dynamics of attractive 1D Bose gases can be much richer than anticipated before because along with condensed states the system supports a new kind of low-lying excited states which are *fragmented*, and thereby not available within the framework of GP theory. These low-lying fragmented excited states are responsible for the formation and evolution of dynamically-stable *fragmented* objects in attractive 1D Bose systems. These objects are distinct from the solitons discussed above.

We solve the time-dependent many-body Schrödinger equation for N attractive bosons in 1D interacting via contact potential $U(x - x') = \lambda_0 \delta(x - x')$ in free space within the framework of the recently developed multi-configurational time-dependent Hartree for bosons (MCTDHB) [9]. For comparison we also integrate the respective time-dependent GP equation. In GP theory the wavefunction has the form $\Psi(x_1, \dots, x_N, t) = \phi_1(x_1, t)\phi_1(x_2, t) \cdots \phi_1(x_N, t)$, i.e., all bosons reside in a single orbital $\phi_1(x, t)$. MCTDHB(M) goes much beyond GP in that the bosons are distributed over M orbitals $\{\phi_i(x, t)\}$ and all possible distributions are considered. The MCTDHB(M) ansatz reads $\Psi(x_1, x_2, \dots, x_N, t) = \sum_{\vec{m}} C_{\vec{m}}(t) \hat{\mathcal{S}} \phi_1(x_1, t) \cdots \phi_2(x_{m_1+1}, t) \cdots \phi_3(x_{m_1+m_2+1}, t) \cdots \phi_M(x_N, t)$ where $\hat{\mathcal{S}}$ is symmetrization operator and $\vec{m} = (m_1, m_2, \dots, m_M)$ occupation numbers. Within this theory a quantitative description of the time evolution of bosonic systems is achieved by optimizing all M orbitals used to construct the many-body expansion and the expansion coefficients them-

selves at each point in time utilizing time-dependent variational principle [9].

At $t=0$ we take as initial condition a *totally condensed* atomic cloud of a very-well defined shape and propagate the many-body MCTDHB(2) and GP equations in time and compare the obtained densities. In this work we take initial coherent wave-packets where all bosons are in either *Sech* $[\gamma x]$ - or Gaussian-shaped normalized functions. These choices represent different ways to generate the initial conditions, leading, however, to similar physical results. Varying the widths of the initial wave packet and keeping the number of bosons and their interparticle interaction strength fixed allows us to change the energy of the initial wave packet and to activate thereby different excited states of the many-boson attractive system. In this study we allow only for initial wave-packets which energetically do not exceed the formation energy of two-hump soliton trains. Thus, *by construction* all the results observed in the present study cannot be attributed to soliton trains.

In Fig. 1 we present the results of the many-body Schrödinger equation for $N=1000$ attractive bosons with $\lambda_0 = -0.008$ for several *Sech*-shaped initial wave-packets of different widths. Here and in the following we work in dimensionless units which are readily arrived at by introducing a convenient length scale L (say, the scattering length) and dividing the Hamiltonian by $\frac{\hbar^2}{mL^2}$, where m is the mass of a boson. The densities are plotted as a function of time. The many-body MCTDHB densities depicted in the left column can be compared with the respective time-dependent GP densities plotted in the right column obtained for the same system with identical initial conditions. The ground eigenstate of the many-boson attractive system in free space at the GP level of description is known analytically – it is the famous *Sech* $[\gamma x]$ with optimal exponent $\gamma = \frac{|\lambda_0|(N-1)}{2}$. For the system under investigation the optimal exponent corresponding to the ground eigenstate is $\gamma \approx 4.0$. In the first study we take a slightly broader initial *Sech*-function with $\gamma_I = 3.0$. The corresponding many-body and GP dynamics are depicted in the upper left and right panels of Fig. 1, respectively. We see that the width of the wave-packet changes in time rather periodically describing thereby ”breathing” of the attractive atomic cloud. The many-body and GP dynamics are quite similar (but not identical) confirming the solitonic character of the ground state also at the many-body level of description. In the second study presented in the middle panels of Fig. 1 we compare many-body and GP dynamics for a broader initial *Sech*-function with $\gamma_{II} = 1.2$. We see that dynamics of the first five ”breathing” oscillations are quite similar within both theories, while at longer times the many-body theory shows attempts of the

density to split into two parts. The bottom panels of Fig. 1 show the results of the third study, where we compare many-body and GP propagations of an even broader initial *Sech*-function with $\gamma_{III} = 1.0$. Again, the first three "breathing" oscillations of the GP dynamics resemble the respective many-body ones, then, however, the many-body dynamics reveal a fascinating feature of the evolution – the initially condensed single *Sech*-shaped cloud dissociates into two smaller equal clouds which move symmetrically apart from each other with approximately constant velocity.

We stress several points. First, the dynamical many-body splitting is a general phenomenon found for many initial conditions and for wave-packets of other shapes as well, e.g., for symmetric and asymmetric Gaussian-shaped profiles. Asymmetric initial packets dissociate into unequal parts. Second, the phenomenon takes place only if the energy of the initial cloud exceeds some threshold value (see below). Third, by increasing the widths of the initial wave packets we increase their total energies making thereby different excited states of the quantum many-boson system energetically accessible. The existence of the splitting phenomenon found only at the many-body level of description indicates that in attractive 1D Bose systems there is a new kind of low-lying excited states, which is not available within the framework of GP theory.

To get a deeper insight into the physics, we investigate next the many-body structures of the evolving wave-packets in some details. By diagonalizing the reduced one-body density matrix at each time step we observe how its eigenvalues, i.e., natural occupation numbers (n_i) and its eigenvectors, i.e., natural orbitals evolve during the dynamics. The evolutions of the natural occupation numbers for all the three initial conditions reported in Fig. 1 are plotted in Fig. 2. We choose log scale to plot the time evolution of the n_i/N in %. At $t=0$ all the bosons of the initial wave-packets reside in one and the same natural orbital indicating that these states, according to the usual definition [10] are condensed. In time we see that another orbital acquires some population revealing the depletion of the initially-condensed state. Interestingly, during the times where the system shows "breathing" dynamics, the changes of the respective natural occupations are moderate. Indeed, for $\gamma_I = 3.0$ where GP theory predicts very similar breathing dynamics, the occupation of the second natural orbital does not exceed 2%. In the other studies ($\gamma_{II} = 1.2, \gamma_{III} = 1.0$) the second natural occupation number oscillatory increases until 10-15% as long as the density exhibits "breathing" oscillations. Then, the system fragments (see Fig. 2).

Let us concentrate on the third study. As time proceeds, the occupation of the second natural orbital increases and around the point where the cloud starts to dissociate into two parts, the two natural occupation numbers become equal and macroscopic. According to the usual definition [11] such a system is two-fold fragmented. Clearly, GP theory is inapplicable here. Further evolution reveals oscillations of the occupation numbers around this ideally two-fold fragmented state. This results from the fact that the respective natural orbitals themselves are delocalized objects, so that even at very large separations the dissociated parts remain connected and can "talk" to each other (see below). The two separated packets propagate almost without dispersion like ordinary solitons (see also Fig. 1). We call this new physical object *fragmenton* because it combines macroscopic fragmentation of the wave function and dynamical properties of a soliton. We recall that in contrast to the ordinary soliton or soliton train solutions which are *coherent* objects, fragmenton is fragmented, i.e., characterized by macroscopic occupations of several (here two) natural orbitals.

For the sake of interpretation, we construct a simple static model which is able to describe two-fold fragmented states $|n_1, n_2\rangle$, where n_1 bosons reside in ϕ_1 and $n_2 = N - n_1$ in ϕ_2 orbitals. As the orbitals constituting this state we choose delocalized gerade and ungerade superpositions of two identical *Sech*-functions with equal exponent γ_m placed at $\pm X_0$ with respect to the origin:

$$\phi_{1,2} = Y_{1,2} [Sech(\gamma_m(x - X_0)) \pm Sech(\gamma_m(x + X_0))], \quad (1)$$

where $Y_{1,2}$ are the respective normalization factors. Our goal is to find within this ansatz the lowest energy eigenstates of the N identical interacting bosons. We consider the exponent γ_m and position X_0 of the *Sech*-functions as variational parameters. Additionally we can change the occupation number n_1 ($n_2 = N - n_1$). The expectation energy of a two-fold fragmented state is known [12]:

$$\begin{aligned} E(n_1) = & n_1 h_{11} + \lambda_0 \frac{n_1(n_1 - 1)}{2} \int |\phi_1|^4 dx + n_2 h_{22} \\ & + \lambda_0 \frac{n_2(n_2 - 1)}{2} \int |\phi_2|^4 dx + 2\lambda_0 n_1 n_2 \int |\phi_1|^2 |\phi_2|^2 dx \end{aligned} \quad (2)$$

where $h_{ii} = \langle \phi_i | -\frac{1}{2} \frac{d^2}{dx^2} | \phi_i \rangle$ are the expectation values of the kinetic energy operator. The minima of this energy functional are plotted in Fig. 3 for our system of $N=1000$ bosons with $\lambda_0 = -0.008$ as a function of n_1 .

The ground state corresponds to the situation where all the bosons are condensed in one localized orbital $|N, 0\rangle$. For an open system this is *exactly* the bright soliton GP solution with $X_0 = 0$ and $\gamma_m \equiv \frac{|\lambda_0|(N-1)}{2}$, which is reproduced by our model. In the right lower corner of Fig. 3 we schematically plot this function. If we increase the population of the second orbital, the total energy of the system increases and the density starts to split, i.e., X_0 has non-zero values. For example for $n_1 = 3N/4$, the minimum energy $E/N = -1.7135$ is obtained for individual *Sech*-functions slightly ($X_0 = 0.2907$) separated from each other and have exponent $\gamma_m = 2.9839$. In Fig. 3 we depict this energy and respective orbitals $\sqrt{n_i/N}\phi_i$. However, our simple model accounts for two branches of physically different solutions. For any given n_1 – there is another branch of solutions which is much higher in energy and characterized by large values of optimal X_0 , i.e., by two very-well separated humps. Indeed, for $n_1 = 3N/4$ such a solution has optimal energy $E/N = -1.2586$ with exponent $\gamma_m = 2.7480$ and separation $X_0 = 4.0$. We depict the respective energy point and pair of orbitals in Fig. 3. Reducing n_1 further, we increase the energy of the lower branch and decrease the energy of the upper branch which approaches its minimum at $n_1 = n_2 = N/2$. At this point, as we can see in Fig. 3, one encounters a bifurcation of the branches. Increasing the occupation of the second orbital further, the energy increases until at $n_1 = 0, n_2 = N$ we arrive at the two-soliton anti-phase (ungerade) solution, plotted in the left upper corner of Fig. 3.

There are three points of relevance indicated in Fig. 3: Ground state (GS), excited state (ES) and the bifurcation point (BF) which corresponds to the ideally fragmented ($n_1 = n_2 = N/2$) state of minimal energy. In our model the optimal energies of all these states have a unique form $E_{state} = -N\gamma_{state}^2/6$, with different optimal exponents γ_{state} . Indeed, the ground state energy of the bright soliton is known: $E_{GP}^{GS} = -N\gamma_{GS}^2/6$ with $\gamma_{GS} = |\lambda_0|(N-1)/2$. The energies of the coherent two-soliton gerade and ungerade states can be obtained by minimizing the GP energy functional assuming zero overlap of the constituting solitons. Then these degenerate energies are $E_{GP}^{ES} = -N\gamma_{ES}^2/6$ with exponent $\gamma_{ES} = |\lambda_0|(N-1)/4$. Finally, assuming that the *Sech*-functions forming the orbitals of ideally fragmented state do not overlap, we get by minimizing Eq. (2) the optimal exponent $\gamma_{BF} = |\lambda_0|(3N/2-1)/4$ and bifurcation energy $E_{BF} = -N\gamma_{BF}^2/6$. From these energies we see that the ideally two-fold fragmented state is separated from the ground state by the energy gap $\Delta E_{FR} \approx 7N^3\lambda_0^2/384$. This energy can be viewed as the threshold for the

activation of the fragmenton. The energy difference between the ground and excited GP states is $\Delta E_{ES} \approx 12N^3\lambda_0^2/384$. Therefore, in attractive one-dimensional Bose gases two-fold fragmented delocalized states are always energetically more favorable than the respective two-soliton coherent gerade and ungerade states.

Now we can interpret the wave-packet evolutions presented in Fig. 1 in terms of the states of the system (see Fig. 3). If the energy of the initial wave-packet relative to the ground state does not exceed the fragmenton activation energy ΔE_{FR} , the model permits dynamics only within the states of the lowest branch. Indeed, in the first study the energy E_I of the initial wave packet (see Fig. 3) is insufficient for activating the fragmenton. The many-body scenario plotted in the left upper panel of Fig. 1 shows small-amplitude "breathing" oscillations around the ground state. In contrast, if the activation threshold is overcome, as it happens in the second (E_{II}) and in particular in the third (E_{III}) study, the fragmenton channel becomes accessible energetically and strongly affects the dynamics. This is reflected in the left middle and lower panels of Fig. 1 where the initial wave packet attempts to split and successfully dissociates into two parts, respectively. The respective E_I , E_{II} and E_{III} energies are shown in Fig. 3.

Let us summarize. We explore the challenging many-body dynamics of attractive ultracold bosonic clouds in 1D by varying the width and thereby the total energy of the initial coherent *Sech*-shaped wave-packet. We solve the many-boson time-dependent Schrödinger equation and show that the many-body dynamics of attractive condensates can differ considerably from the respective GP dynamics. We find that when the initial energy of the condensate exceeds some threshold, the condensed cloud at the many-body level of description tends to split and can dynamically dissociate into two separate parts, while at the GP level it reveals only "breathing" dynamics and remains unsplit. To understand this phenomenon we first analyze the many-body wave-function and attribute the split clouds to a two-fold fragmented delocalized state. We call this new class of dynamical solutions *fragmentons* because on the one hand they propagate almost without dispersion, and on the other hand, in contrast to solitons, they are not coherent objects. A simple static model is introduced to show that the two-fold fragmented state constructed from in- and anti- phase two-soliton-like functions is energetically much more favorable than coherent two-soliton solutions. To estimate the window for fragmenton formation we provide simple estimations of the energies of the involved states in terms of the number of particles N and their interaction

strength λ_0 .

Our findings imply that the dynamics of attractive Bose gases in low dimensions is much richer than anticipated before and we hope that our work will stimulate experiments on fragmentons.

Acknowledgments

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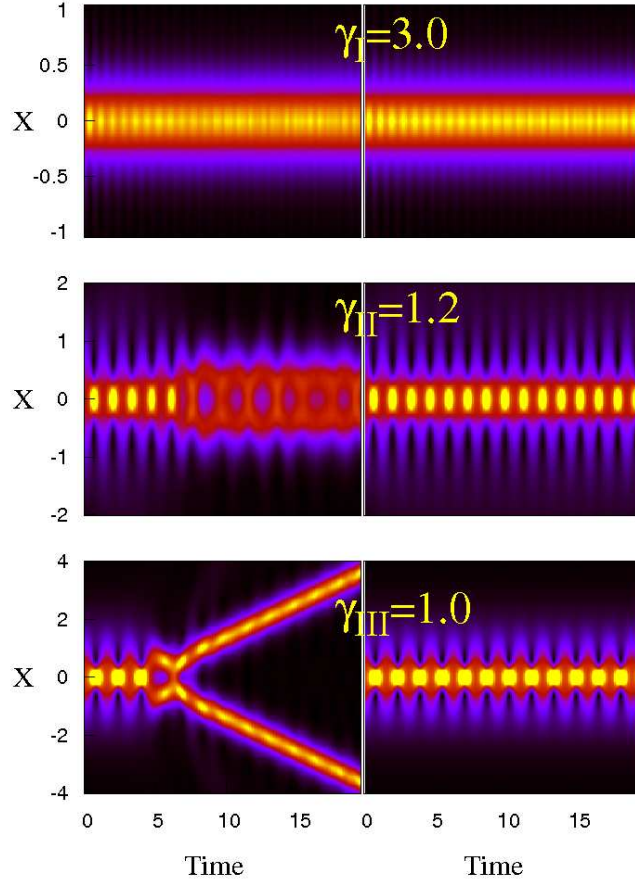


FIG. 1: (Color online) MCTDHB many-body (left) vs. GP (right) dynamics for $N=1000$ attractive ($\lambda_0 = -0.008$) bosons in one-dimension. The densities are plotted as a function of time for initially-coherent wave-packets $Sech[\gamma x]$ of different widths. While the GP dynamics shows "breathing" oscillations for all initial widths, the many-body dynamics changes dramatically from "breathing" oscillations ($\gamma_I = 3.0$), to attempts for dynamical splitting ($\gamma_{II} = 1.2$), and to dynamical dissociation into two parts ($\gamma_{III} = 1.0$). All quantities are dimensionless.

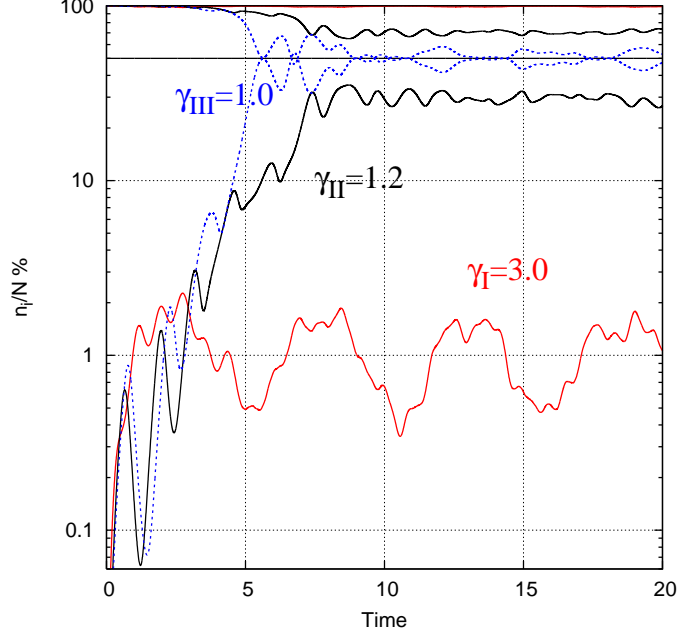


FIG. 2: (Color online) Evolutions of natural occupation numbers n_1/N and n_2/N of the reduced one-body densities plotted in the left panels of Fig. 1 on a log scale in %. At $t=0$ all initial states are condensed: $n_1/N = 100\%$. In the first study ($\gamma_I = 3.0$) the dynamics describe "breathing" oscillations only. In the second ($\gamma_{II} = 1.2$) and third ($\gamma_{III} = 1.0$) studies the systems evolve to be two-fold fragmented after few "breathing" oscillations. Notice that in GP n_1/N is always 100 %. All quantities are dimensionless.

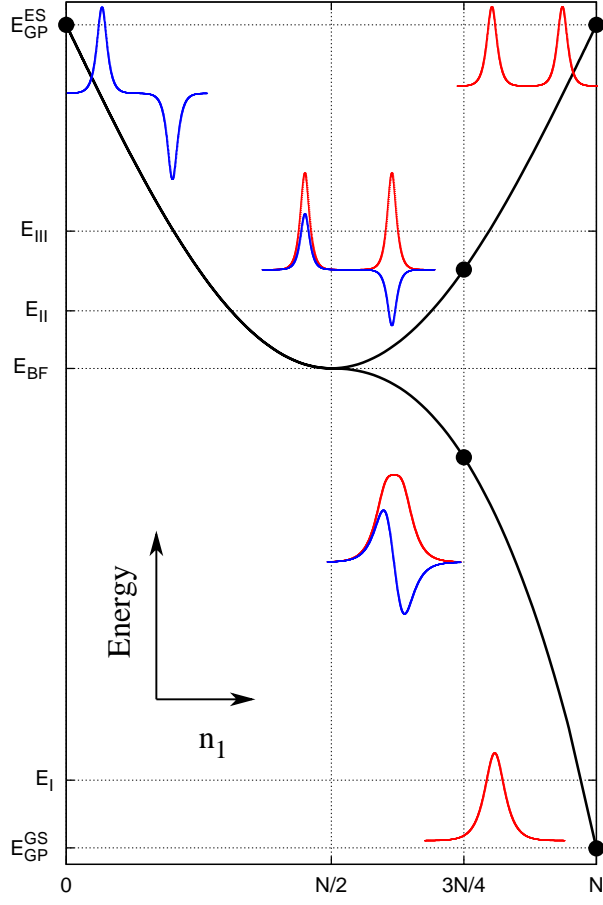


FIG. 3: (Color online) Energy diagram $E(n_1)$ of the model system introduced in Eqs. (1,2) for two-fold fragmented $|n_1, n_2\rangle$ states $n_1 + n_2 = N$. There are two branches of solutions bifurcating at $n_1 = N/2$ (bifurcation energy E_{BF}). Shown are also the orbitals $\sqrt{n_i/N}\phi_i$ corresponding to $n_1 = 3N/4$ at both branches and to the GP solutions of $n_1 = N$ and $n_2 = N$ at energies E_{GP}^{GS} and E_{GP}^{ES} . E_I, E_{II}, E_{III} are the energies of the three cases studied in Fig. 1. To activate a fragmenton the energy of the initial cloud must exceed E_{BF} . All quantities are dimensionless.